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=> d his

     (FILE 'HOME' ENTERED AT 21:50:18 ON 17 JUL 2003)

     FILE 'REGISTRY' ENTERED AT 21:50:28 ON 17 JUL 2003
L1              STRUCTURE UPLOADED
L2            0 S L1
L3            2 S L1 FULL

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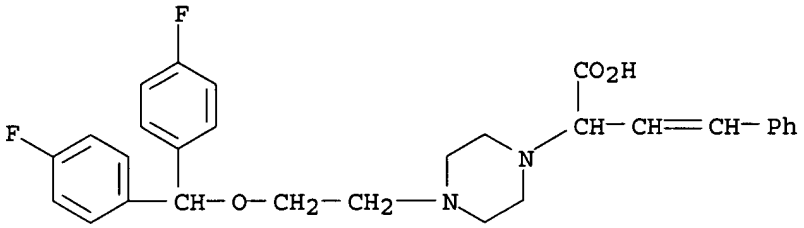
=> d all 1-
YOU HAVE REQUESTED DATA FROM 2 ANSWERS - CONTINUE? Y/(N):y

L3 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 350583-56-1 REGISTRY
CN 1-Piperazineacetic acid,
4-[2-[bis(4-fluorophenyl)methoxy]ethyl]-.alpha.-(2-phenylethenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H30 F2 N2 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	3
C4N2	NC2NC2	6	C4N2	46.383.1	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	18.0	pH 1	(1) ACD
Bioconc. Factor (BCF)	137	pH 4	(1) ACD
Bioconc. Factor (BCF)	160	pH 7	(1) ACD
Bioconc. Factor (BCF)	125	pH 8	(1) ACD
Bioconc. Factor (BCF)	8.85	pH 10	(1) ACD
Boiling Point (BP)	623.1+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	97.02+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	330.6+/-56.7 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	28.6	pH 1	(1) ACD
Koc (KOC)	218	pH 4	(1) ACD
Koc (KOC)	255	pH 7	(1) ACD
Koc (KOC)	200	pH 8	(1) ACD
Koc (KOC)	14.1	pH 10	(1) ACD
logD (LOGD)	3.05	pH 1	(1) ACD
logD (LOGD)	3.93	pH 4	(1) ACD
logD (LOGD)	4.00	pH 7	(1) ACD
logD (LOGD)	3.89	pH 8	(1) ACD
logD (LOGD)	2.74	pH 10	(1) ACD
logP (LOGP)	6.503+/-0.668		(1) ACD

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	492.56		(1) ACD
pKa (PKA)	3.93+/-0.10	Most Acidic	(1) ACD
pKa (PKA)	8.47+/-0.50	Most Basic	(1) ACD
Vapor Pressure (VP)	2.19E-16 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 135:107255 CA
TI Preparation of polypharmacophoric agents
IN Hanson, Robert N.; Babich, John W.
PA Biostream Therapeutics, Inc., USA
SO PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D241-04
ICS C07D211-34; C07D211-44; C07D223-26
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001051474	A2	20010719	WO 2001-US1035	20010111
	WO 2001051474	A3	20011206		
	W: CA, JP				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
	US 2002042357	A1	20020411	US 2001-758957	20010111
	EP 1257541	A2	20021120	EP 2001-902026	20010111
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
	JP 2003519689	T2	20030624	JP 2001-551856	20010111
PRAI	US 2000-175617P		20000111		
	WO 2001-US1035		20010111		

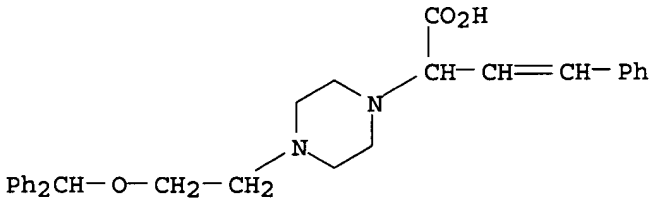
AB Title compds. (I) comprise a scaffold bearing .gtoreq.2 pharmacophore units selected from D1, D2, D3, and D4 agonists, (ir)reversible monoamine inhibitors, monoamine transporter inhibitors, COMT inhibitors, MAO inhibitors, and dopamine transporter inhibitors. I interact with .gtoreq.2 biol. targets. Thus, (E)-PhZCH(CO2H)CH:CHPh (Z = piperidine-4,1-diyl) was prepd. Data for biol. activity of I were given.
ST polypharmacophoric agent prepn; dopaminergic system agent prepn
IT Dopamine agonists
(D1; prepn. of polypharmacophoric agents)
IT Dopamine agonists
(D2; prepn. of polypharmacophoric agents)
IT Dopamine agonists
(D3; prepn. of polypharmacophoric agents)
IT Nervous system
(Huntington's chorea, treatment; prepn. of polypharmacophoric agents)
IT Mental disorder
(attention deficit disorder, treatment; prepn. of polypharmacophoric agents)

IT Mental disorder
(autism, treatment; prepn. of polypharmacophoric agents)
IT Transport proteins
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC
(Process)
(dopamine-transporting, inhibitors; prepn. of polypharmacophoric agents)
IT Nervous system
(dopaminergic; prepn. of polypharmacophoric agents)
IT Monoamines
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC
(Process)
(inhibitors; prepn. of polypharmacophoric agents)
IT Transport proteins
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC
(Process)
(monoamine-transporting, inhibitors; prepn. of polypharmacophoric agents)
IT Anti-inflammatory agents
Antidepressants
Antiobesity agents
Pharmacophores
(prepn. of polypharmacophoric agents)
IT Alzheimer's disease
(treatment; prepn. of polypharmacophoric agents)
IT 9001-66-5, monoamine oxidase 9012-25-3, Catechol O-methyl transferase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC
(Process)
(inhibitors; prepn. of polypharmacophoric agents)
IT 67469-69-6P 350583-53-8P 350583-56-1P 350583-58-3P 350583-59-4P 350583-60-7P 350583-61-8P
350583-62-9P 350583-63-0P 350583-64-1P 350583-65-2P 350583-66-3P 350583-67-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of polypharmacophoric agents)

L3 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 350583-53-8 REGISTRY
CN 1-Piperazineacetic acid,
4-[2-(diphenylmethoxy)ethyl]-.alpha.-(2-phenylethenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H32 N2 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	3
C4N2	NC2NC2	6	C4N2	46.383.1	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	14.9	pH 1	(1) ACD
Bioconc. Factor (BCF)	112	pH 4	(1) ACD
Bioconc. Factor (BCF)	134	pH 7	(1) ACD
Bioconc. Factor (BCF)	105	pH 8	(1) ACD
Bioconc. Factor (BCF)	7.50	pH 10	(1) ACD
Boiling Point (BP)	621.5+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	96.80+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	329.6+/-56.7 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	24.9	pH 1	(1) ACD
Koc (KOC)	188	pH 4	(1) ACD
Koc (KOC)	224	pH 7	(1) ACD
Koc (KOC)	177	pH 8	(1) ACD
Koc (KOC)	12.6	pH 10	(1) ACD
logD (LOGD)	2.94	pH 1	(1) ACD
logD (LOGD)	3.82	pH 4	(1) ACD
logD (LOGD)	3.89	pH 7	(1) ACD
logD (LOGD)	3.79	pH 8	(1) ACD
logD (LOGD)	2.64	pH 10	(1) ACD
logP (LOGP)	6.400+/-0.547		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	456.58		(1) ACD
pKa (PKA)	3.93+/-0.10	Most Acidic	(1) ACD
pKa (PKA)	8.48+/-0.50	Most Basic	(1) ACD
Vapor Pressure (VP)	2.64E-16 Torr	25.0 deg C	(1) ACD

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DT Patent
LA English

IC ICM C07D241-04
ICS C07D211-34; C07D211-44; C07D223-26
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	EP 1257541	A2	20021120	EP 2001-902026	20010111
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IT Dopamine agonists
(D3; prepn. of polypharmacophoric agents)
IT Nervous system
(Huntington's chorea, treatment; prepn. of polypharmacophoric agents)
IT Mental disorder
(attention deficit disorder, treatment; prepn. of polypharmacophoric agents)
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IT Transport proteins
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Pharmacophores
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IT Alzheimer's disease
(treatment; prepn. of polypharmacophoric agents)

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350583-62-9P 350583-63-0P 350583-64-1P 350583-65-2P 350583-66-3P 350583-67-4P
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(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
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